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computer program abstracts

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PSEUDO: a program for a pseudo-symmetry search

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1. The crystallographic problem

The program *PSEUDO* provides tools for the systematic search of pseudosymmetry, based on group–subgroup relations between space groups (Igartua *et al.*, 1996). For a crystal structure **L**, specified by its space group U, the cell parameters and the coordinates of the atoms in the asymmetric unit, the program searches for pseudosymmetry among all minimal supergroups $G_k > U$ of the group U. The interpretation of a structural pseudosymmetry as a small distortion of a higher symmetric (prototype) structure **H** allows the following.

(i) The prediction of phase transitions at higher temperature. If the distortion is small enough, it can be expected that the crystal acquires the more symmetric configuration at a higher temperature after a phase transition (Igartua *et al.*, 1996, 1999).

(ii) The search for new ferroelastic and ferroelectric materials. Polar structures having atomic displacements smaller than 1 Å with respect to a hypothetical non-polar configuration are considered as possible ferroelectrics (Abrahams & Keve, 1971; Kroumova *et al.*, 2000).

(iii) The detection of false symmetry assignments (overlooked symmetry) in crystal structure determination.

2. Method of solution

The procedure is based on the assumption that the symmetry of the prototype structure **H** is described by a supergroup $G > U$. As any group–subgroup chain can be represented by a chain of minimal supergroups, the search for pseudosymmetry is restricted to the minimal supergroups $G_k > U$ of U, which are determined in the first step. In the case of non-polar space groups U, the number k is finite and small if the isomorphic supergroups are limited to those of small index (which is a physically reasonable assumption).

Once the minimal supergroups G_k are derived, the pseudosymmetry search is carried out by a straightforward checking of the compatibility of the additional symmetry elements of all groups G_k with the initial crystal structure. For that it is sufficient to compare the crystal structure **L** with its variants obtained by transformations of **L** with all representatives of the coset decomposition of G_k relative to U. A structure **L** is considered pseudosymmetric if all atoms in the structure deviate from their ideal positions in **H** by less than some previously determined tolerance factor, *e.g.* 1 Å.

The main difficulty in the generalization of the pseudosymmetry procedure for the case of ferroelectrics arises from the infinite number of minimal non-polar supergroups of polar space groups. In practice, this implies that there are no restrictions on the locations of the additional pseudosymmetry elements (inversion centre, plane or binary axis) relative to the polar initial structure. This means that the coset representatives of the non-polar supergroup G relative to the polar space group U contain one or more continuous parameters ε in the translational part, which have to be optimized using structural criteria. In the program, the pseudosymmetry is checked, optimizing ε by minimization of the resulting atomic displacements necessary to obtain the high-symmetry structure.

3. Software and hardware environment

The program *PSEUDO* runs under any Unix or Unix-like operating system (Digital Unix, HP-UX, Sun, BSD, Linux, *etc.*). *PSEUDO* is written in C and Perl. Only standard library functions are used. No overlay structure has been applied.

The program runs on any computer with Unix operating system (Intel, Alpha, Sparc, Mips, *etc.*). The amount of memory used depends on the complexity of the initial structure. *PSEUDO* can be used without local installation from any computer with a Web browser (Unix, VMS, Macintosh, DOS, Windows, *etc.*) as it forms part of the Bilbao Crystallographic Server (Kroumova *et al.*, 1998, 1999).

4. Program specifications

As input, the program requires the crystal structure **L**, specified by its space group U (given by the number in the *International Tables for Crystallography*, Vol. *A*), the cell parameters and the positions of the atoms in the asymmetric unit. If these are referred to a non-conventional coordinate system, the data for the change of basis and the origin shift have to be added. The user can choose the tolerance factor, which limits the maximal atomic displacements with respect to the high-symmetry prototype structure.

The output from the program contains the pseudosymmetry supergroups G_k determined by their coset representatives relative to U, the relations between the atoms in the initial and the transformed structure, the atomic displacements necessary to obtain the structure **H** from **L**, and the ideal atomic positions of the atoms in **H**.

5. Documentation

An on-line description of the input for and the output of the program is available at http://www.cryst.ehu.es/cryst/pseudo/help.html. The

description of the method can be found at http://www.cryst.ehu.es/cryst/pseudo/doc.html.

6. Availability

The program forms part of the Bilbao Crystallographic Server, http://www.cryst.ehu.es, and uses the databases and the results from other programs available on this server. *PSEUDO* can be used from any computer with a Web browser *via* the Internet. The URL of the program is http://www.cryst.ehu.es/cryst/pseudo.html.

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